



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 05:25 pm BST

PDB ID : 5GJ7
Title : putative Acyl-CoA dehydrogenase
Authors : Moon, H.; Choe, J.
Deposited on : 2016-06-28
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

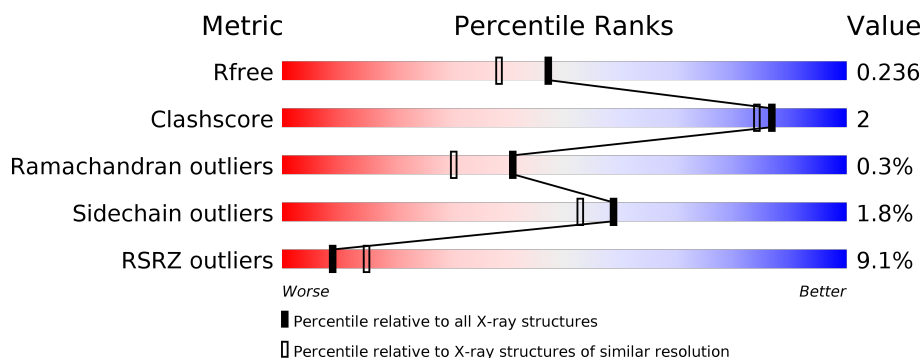
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	398	<div> <div>7%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>• •</div> </div> </div>
1	B	398	<div> <div>11%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6313 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Acyl-CoA dehydrogenase type 2 domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			3021	1912	539	558	12			
1	B	388	Total	C	N	O	S	0	0	0
			3021	1912	539	558	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP C8WV06
A	-1	ASN	-	expression tag	UNP C8WV06
A	0	ALA	-	expression tag	UNP C8WV06
B	-2	SER	-	expression tag	UNP C8WV06
B	-1	ASN	-	expression tag	UNP C8WV06
B	0	ALA	-	expression tag	UNP C8WV06

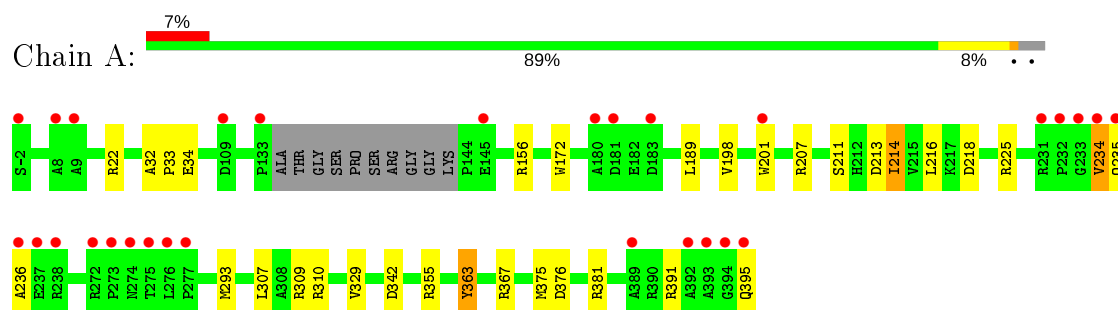
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	161	Total	O	0	0
			161	161		
2	B	110	Total	O	0	0
			110	110		

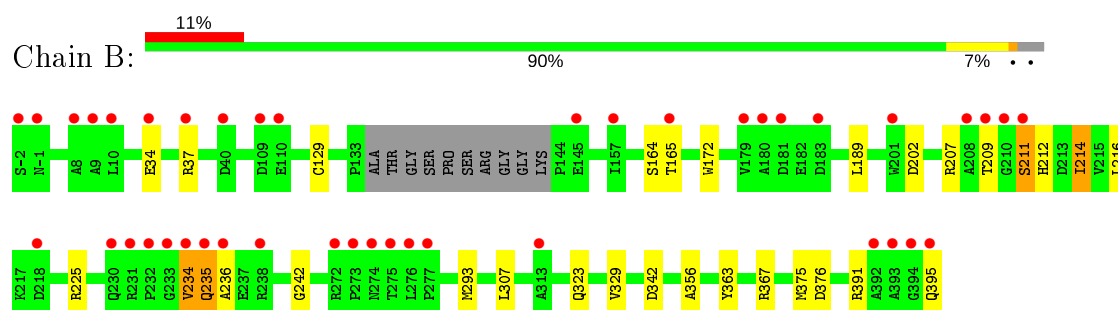
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Acyl-CoA dehydrogenase type 2 domain protein



- Molecule 1: Acyl-CoA dehydrogenase type 2 domain protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	155.69 Å 69.38 Å 83.25 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95 19.88 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-1.95) 99.2 (19.88-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.22 (at 1.96 Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.196 , 0.224 0.210 , 0.236	Depositor DCC
R_{free} test set	3318 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6313	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.82 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4818e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.83	1/3084 (0.0%)	0.91	13/4190 (0.3%)
1	B	0.77	0/3084	0.89	7/4190 (0.2%)
All	All	0.80	1/6168 (0.0%)	0.90	20/8380 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	GLU	CD-OE1	6.42	1.32	1.25

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	MET	CG-SD-CE	-7.60	88.04	100.20
1	A	225	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	B	293	MET	CG-SD-CE	-7.23	88.63	100.20
1	A	342	ASP	CB-CG-OD1	7.21	124.79	118.30
1	A	225	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	B	342	ASP	CB-CG-OD1	6.52	124.17	118.30
1	A	391	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	B	225	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	B	225	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	B	376	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	309	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	B	207	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	376	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	381	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	A	381	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	22	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	391	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	207	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	363	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	A	310	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3021	0	3026	13	0
1	B	3021	0	3026	16	0
2	A	161	0	0	0	0
2	B	110	0	0	0	0
All	All	6313	0	6052	25	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (25) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:THR:O	1:B:209:THR:OG1	2.00	0.79
1:B:211:SER:O	1:B:212:HIS:HD2	1.86	0.59
1:B:234:VAL:HG23	1:B:235:GLN:HA	1.85	0.58
1:A:234:VAL:HG23	1:A:235:GLN:HA	1.89	0.55
1:A:307:LEU:HD12	1:A:329:VAL:CG2	2.38	0.53
1:B:307:LEU:HD12	1:B:329:VAL:CG2	2.41	0.50
1:B:34:GLU:HG3	1:B:37:ARG:HH22	1.77	0.49
1:A:156:ARG:HD2	1:A:218:ASP:OD1	2.13	0.49
1:A:214:ILE:HD11	1:A:216:LEU:HD11	1.95	0.48
1:B:211:SER:O	1:B:212:HIS:CD2	2.66	0.48
1:B:214:ILE:HD11	1:B:216:LEU:HD11	1.96	0.48
1:A:307:LEU:CD1	1:A:329:VAL:CG2	2.93	0.47
1:A:355:ARG:HD3	1:B:202:ASP:OD2	2.17	0.45
1:B:307:LEU:CD1	1:B:329:VAL:CG2	2.95	0.44
1:A:201:TRP:CD2	1:B:356:ALA:HB2	2.53	0.43
1:A:32:ALA:N	1:A:33:PRO:CD	2.82	0.42
1:B:129:CYS:SG	1:B:164:SER:HB3	2.59	0.42
1:A:363:TYR:CZ	1:B:367:ARG:HD3	2.55	0.42
1:B:164:SER:OG	1:B:214:ILE:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:VAL:CG2	1:A:213:ASP:HB2	2.49	0.42
1:A:367:ARG:HD3	1:B:363:TYR:CZ	2.56	0.41
1:B:172:TRP:HB3	1:B:189:LEU:HD11	2.02	0.41
1:B:242:GLY:O	1:B:323:GLN:HG2	2.20	0.41
1:A:307:LEU:CD1	1:A:329:VAL:HG23	2.50	0.40
1:A:172:TRP:HB3	1:A:189:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	384/398 (96%)	381 (99%)	2 (0%)	1 (0%)	41	30
1	B	384/398 (96%)	381 (99%)	2 (0%)	1 (0%)	41	30
All	All	768/796 (96%)	762 (99%)	4 (0%)	2 (0%)	41	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	236	ALA
1	A	236	ALA

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	313/319 (98%)	308 (98%)	5 (2%)	62	58
1	B	313/319 (98%)	307 (98%)	6 (2%)	57	50
All	All	626/638 (98%)	615 (98%)	11 (2%)	59	53

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	SER
1	A	214	ILE
1	A	234	VAL
1	A	375	MET
1	A	395	GLN
1	B	211	SER
1	B	214	ILE
1	B	234	VAL
1	B	235	GLN
1	B	375	MET
1	B	395	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	248	HIS
1	A	325	GLN
1	A	371	HIS
1	B	212	HIS
1	B	325	GLN
1	B	371	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	388/398 (97%)	0.35	29 (7%) 14 22	17, 29, 64, 119	0
1	B	388/398 (97%)	0.60	42 (10%) 5 9	18, 34, 75, 145	0
All	All	776/796 (97%)	0.48	71 (9%) 9 15	17, 32, 72, 145	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	234	VAL	16.8
1	B	233	GLY	9.5
1	B	211	SER	8.5
1	A	235	GLN	7.8
1	A	233	GLY	7.7
1	B	232	PRO	7.7
1	A	234	VAL	6.7
1	B	235	GLN	6.5
1	B	210	GLY	6.3
1	A	274	ASN	6.2
1	A	181	ASP	5.9
1	A	232	PRO	5.9
1	A	394	GLY	5.5
1	B	394	GLY	5.4
1	A	201	TRP	5.4
1	B	277	PRO	5.4
1	B	181	ASP	5.3
1	B	274	ASN	5.2
1	A	275	THR	5.2
1	B	201	TRP	4.9
1	B	209	THR	4.8
1	B	275	THR	4.6
1	A	183	ASP	4.6
1	B	393	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	395	GLN	4.2
1	A	395	GLN	4.1
1	A	272	ARG	4.1
1	A	276	LEU	4.0
1	B	236	ALA	4.0
1	A	277	PRO	3.9
1	A	236	ALA	3.8
1	B	-2	SER	3.8
1	A	8	ALA	3.5
1	B	183	ASP	3.4
1	B	8	ALA	3.4
1	A	392	ALA	3.2
1	B	208	ALA	3.1
1	B	276	LEU	3.1
1	B	238	ARG	3.0
1	B	145	GLU	3.0
1	B	231	ARG	3.0
1	A	9	ALA	3.0
1	B	40	ASP	3.0
1	B	157	ILE	2.9
1	B	165	THR	2.8
1	B	272	ARG	2.8
1	A	393	ALA	2.7
1	A	133	PRO	2.7
1	A	238	ARG	2.7
1	B	9	ALA	2.6
1	B	392	ALA	2.6
1	A	180	ALA	2.6
1	B	180	ALA	2.6
1	B	37	ARG	2.5
1	A	231	ARG	2.4
1	B	-1	ASN	2.4
1	A	273	PRO	2.4
1	B	110	GLU	2.3
1	B	179	VAL	2.3
1	B	273	PRO	2.3
1	B	109	ASP	2.3
1	B	230	GLN	2.2
1	A	-2	SER	2.2
1	A	145	GLU	2.2
1	A	237	GLU	2.2
1	B	218	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	10	LEU	2.2
1	B	34	GLU	2.1
1	B	313	ALA	2.1
1	A	389	ALA	2.1
1	A	109	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.